

Substance Name	CASRN	Lab Number	In Vitro Concentration Tested	In Vitro Physical Form Tested	Purity (%)	Solubility ¹	pH	Q-Score ²	Q-Score Classification	Overall Q-Score Classification	Reference
Acetone	67-64-1	1	100%	Liquid	>99	water soluble		18.36	Severe	Severe	Balls et al. (1995)
Acetone	67-64-1	2	100%	Liquid	>99	water soluble		13.53	Severe		Balls et al. (1995)
Acetone	67-64-1	3	100%	Liquid	>99	water soluble		0.80	Nonirritant		Balls et al. (1995)
Acetone	67-64-1	4	100%	Liquid	>99	water soluble		10.31	Severe		Balls et al. (1995)
Ammonium nitrate	6484-52-2	1	100%	Solid	>99.9	water soluble		1.80	Moderate	Moderate	Balls et al. (1995)
Ammonium nitrate	6484-52-2	3	100%	Solid	>99.9	water soluble		1.30	Nonirritant		Balls et al. (1995)
L-Aspartic acid	70-47-3	1	100%	Solid	95	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	1%	Solution	98	surfactant		3.41	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	1%	Solution	98	surfactant		5.00	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	1%	Solution	98	surfactant		3.90	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	1%	Solution	98	surfactant		4.39	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	5%	Solution	98	surfactant		6.93	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	5%	Solution	98	surfactant		4.43	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	5%	Solution	98	surfactant		1.20	Nonirritant		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	5%	Solution	98	surfactant		6.49	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	1	10%	Solution	98	surfactant		6.09	Severe	Severe	Balls et al. (1995)
Benzalkonium chloride	8001-54-5	2	10%	Solution	98	surfactant		7.03	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	3	10%	Solution	98	surfactant		3.10	Severe		Balls et al. (1995)
Benzalkonium chloride	8001-54-5	4	10%	Solution	98	surfactant		6.14	Severe		Balls et al. (1995)
Butyl acetate	123-86-4	1	100%	Liquid	99	water insoluble		1.55	Moderate	Moderate	Balls et al. (1995)
Butyl acetate	123-86-4	2	100%	Liquid	99	water insoluble		1.23	Nonirritant		Balls et al. (1995)
Butyl acetate	123-86-4	3	100%	Liquid	99	water insoluble		1.80	Moderate		Balls et al. (1995)
Butyl acetate	123-86-4	4	100%	Liquid	99	water insoluble		1.93	Moderate		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	1	100%	Liquid	>99	water soluble		22.04	Severe	Severe	Balls et al. (1995)
Gamma-butyrolactone	96-48-0	2	100%	Liquid	>99	water soluble		6.64	Severe		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	3	100%	Liquid	>99	water soluble		1.97	Moderate		Balls et al. (1995)
Gamma-butyrolactone	96-48-0	4	100%	Liquid	>99	water soluble		4.02	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	0.10%	Solution	98	surfactant		2.43	Severe	Nonirritant	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	0.10%	Solution	98	surfactant		0.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	0.10%	Solution	98	surfactant		1.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	0.10%	Solution	98	surfactant		0.00	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	1	6%	Solution	98	surfactant		2.34	Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	6%	Solution	98	surfactant		2.42	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	6%	Solution	98	surfactant		1.30	Nonirritant		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	6%	Solution	98	surfactant		3.11	Severe		Balls et al. (1995)

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Cetylpyridinium bromide	140-72-7	1	10%	Solution	98	surfactant		2.71	Severe	Severe	Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	2	10%	Solution	98	surfactant		2.73	Severe		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	3	10%	Solution	98	surfactant		1.80	Moderate		Balls et al. (1995)
Cetylpyridinium bromide	140-72-7	4	10%	Solution	98	surfactant		4.67	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	1	100%	Liquid	97	water soluble		3.28	Severe	Severe	Balls et al. (1995)
Cyclohexanol	108-93-0	2	100%	Liquid	97	water soluble		4.48	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	3	100%	Liquid	97	water soluble		5.20	Severe		Balls et al. (1995)
Cyclohexanol	108-93-0	4	100%	Liquid	97	water soluble		6.69	Severe		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	1	100%	Liquid	99	water insoluble		10.14	Severe	Severe	Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	2	100%	Liquid	99	water insoluble		8.81	Severe		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	3	100%	Liquid	99	water insoluble		1.90	Moderate		Balls et al. (1995)
2,6-Dichlorobenzoyl chloride	4659-45-4	4	100%	Liquid	99	water insoluble		2.53	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	1	100%	Liquid	>99	water insoluble		14.05	Severe	Severe	Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	2	100%	Liquid	>99	water insoluble		10.64	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	3	100%	Liquid	>99	water insoluble		11.70	Severe		Balls et al. (1995)
2,2-Dimethylbutanoic acid	595-37-9	4	100%	Liquid	>99	water insoluble		14.73	Severe		Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	1	100%	Solid	99.5	water insoluble		2.07	Severe	Severe	Balls et al. (1995)
2,5-Dimethylhexanediol	110-03-2	3	100%	Solid	99.5	water insoluble		0.80	Nonirritant		Balls et al. (1995)

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Ethanol	64-17-5	1	100%	Liquid		water soluble		6.45	Severe	Severe	Balls et al. (1995)
Ethanol	64-17-5	2	100%	Liquid		water soluble		10.63	Severe		Balls et al. (1995)
Ethanol	64-17-5	3	100%	Liquid		water soluble		1.47	Nonirritant		Balls et al. (1995)
Ethanol	64-17-5	4	100%	Liquid		water soluble		5.95	Severe		Balls et al. (1995)
Ethyl acetate	141-78-6	1	100%	Liquid	99	water soluble		3.94	Severe	Severe	Balls et al. (1995)
Ethyl acetate	141-78-6	2	100%	Liquid	99	water soluble		1.87	Moderate		Balls et al. (1995)
Ethyl acetate	141-78-6	3	100%	Liquid	99	water soluble		0.90	Nonirritant		Balls et al. (1995)
Ethyl acetate	141-78-6	4	100%	Liquid	99	water soluble		3.37	Severe		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	1	100%	Liquid	99	water soluble		1.24	Nonirritant	Nonirritant	Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	2	100%	Liquid	99	water soluble		0.61	Nonirritant		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	3	100%	Liquid	99	water soluble		1.00	Nonirritant		Balls et al. (1995)
2-Ethyl-1-hexanol	104-76-7	4	100%	Liquid	99	water soluble		3.12	Severe		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	1	100%	Liquid	ca. 97	water soluble		2.40	Severe	Severe	Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	2	100%	Liquid	ca. 97	water soluble		2.51	Severe		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	3	100%	Liquid	ca. 97	water soluble		1.10	Nonirritant		Balls et al. (1995)
Ethyl-2-methylacetoacetate	609-14-3	4	100%	Liquid	ca. 97	water soluble		2.35	Severe		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	1	100%	Liquid	99	water insoluble		0.10	Nonirritant	Nonirritant	Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	2	100%	Liquid	99	water insoluble		0.19	Nonirritant		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	3	100%	Liquid	99	water insoluble		0.30	Nonirritant		Balls et al. (1995)
Ethyl trimethyl acetate	3938-95-2	4	100%	Liquid	99	water insoluble		1.01	Nonirritant		Balls et al. (1995)

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Glycerol	56-81-5	1	100%	Liquid	>99.5	water soluble		0.08	Nonirritant	Nonirritant	Balls et al. (1995)
Glycerol	56-81-5	2	100%	Liquid	>99.5	water soluble		1.24	Nonirritant		Balls et al. (1995)
Glycerol	56-81-5	3	100%	Liquid	>99.5	water soluble		0.60	Nonirritant		Balls et al. (1995)
Glycerol	56-81-5	4	100%	Liquid	>99.5	water soluble		1.22	Nonirritant		Balls et al. (1995)
Hexanol	111-27-3	1	100%	Liquid	98	water insoluble		5.01	Severe	Severe	Balls et al. (1995)
Hexanol	111-27-3	2	100%	Liquid	98	water insoluble		3.98	Severe		Balls et al. (1995)
Hexanol	111-27-3	3	100%	Liquid	98	water insoluble		1.80	Moderate		Balls et al. (1995)
Hexanol	111-27-3	4	100%	Liquid	98	water insoluble		4.71	Severe		Balls et al. (1995)
Imidazole	288-32-4	1	100%	Solid	99	water soluble		11.19	Severe	Severe	Balls et al. (1995)
Imidazole	288-32-4	3	100%	Solid	99	water soluble		3.50	Severe		Balls et al. (1995)
Isobutanol	78-83-1	1	100%	Liquid	99.9	water insoluble		4.59	Severe	Severe	Balls et al. (1995)
Isobutanol	78-83-1	2	100%	Liquid	99.9	water insoluble		3.58	Severe		Balls et al. (1995)
Isobutanol	78-83-1	3	100%	Liquid	99.9	water insoluble		1.20	Nonirritant		Balls et al. (1995)
Isobutanol	78-83-1	4	100%	Liquid	99.9	water insoluble		5.89	Severe		Balls et al. (1995)
Isopropanol	67-63-0	1	100%	Liquid	99.9	water soluble		11.90	Severe	Severe	Balls et al. (1995)
Isopropanol	67-63-0	2	100%	Liquid	99.9	water soluble		5.79	Severe		Balls et al. (1995)
Isopropanol	67-63-0	3	100%	Liquid	99.9	water soluble		1.80	Moderate		Balls et al. (1995)
Isopropanol	67-63-0	4	100%	Liquid	99.9	water soluble		4.36	Severe		Balls et al. (1995)
Maneb	12427-38-2	1	100%	Solid	90	water soluble		0.00	Nonirritant	Nonirritant	Balls et al. (1995)

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Methyl acetate	79-20-9	1	100%	Liquid	98	water soluble		1.88	Moderate	Severe	Balls et al. (1995)
Methyl acetate	79-20-9	2	100%	Liquid	98	water soluble		5.39	Severe		Balls et al. (1995)
Methyl acetate	79-20-9	3	100%	Liquid	98	water soluble		1.70	Moderate		Balls et al. (1995)
Methyl acetate	79-20-9	4	100%	Liquid	98	water soluble		3.15	Severe		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	1	100%	Liquid	99	water soluble		1.51	Moderate	Moderate	Balls et al. (1995)
Methyl cyanoacetate	105-34-0	2	100%	Liquid	99	water soluble		1.21	Nonirritant		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	3	100%	Liquid	99	water soluble		1.00	Nonirritant		Balls et al. (1995)
Methyl cyanoacetate	105-34-0	4	100%	Liquid	99	water soluble		1.78	Moderate		Balls et al. (1995)
Methylcyclopentane	96-37-7	1	100%	Liquid	>99	water insoluble		0.18	Nonirritant	Nonirritant	Balls et al. (1995)
Methylcyclopentane	96-37-7	2	100%	Liquid	>99	water insoluble		1.22	Nonirritant		Balls et al. (1995)
Methylcyclopentane	96-37-7	3	100%	Liquid	>99	water insoluble		0.20	Nonirritant		Balls et al. (1995)
Methylcyclopentane	96-37-7	4	100%	Liquid	>99	water insoluble		8.09	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	1	100%	Liquid	99	water soluble		5.83	Severe	Severe	Balls et al. (1995)
Methyl ethyl ketone	78-93-3	2	100%	Liquid	99	water soluble		3.89	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	3	100%	Liquid	99	water soluble		2.50	Severe		Balls et al. (1995)
Methyl ethyl ketone	78-93-3	4	100%	Liquid	99	water soluble		6.17	Severe		Balls et al. (1995)

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Methyl isobutyl ketone	108-10-1	1	100%	Liquid	98	water insoluble		2.29	Severe	Moderate	Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	2	100%	Liquid	98	water insoluble		1.04	Nonirritant		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	3	100%	Liquid	98	water insoluble		1.50	Moderate		Balls et al. (1995)
Methyl isobutyl ketone	108-10-1	4	100%	Liquid	98	water insoluble		1.86	Moderate		Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	1	100%	Solid	95	water soluble		3.84	Severe	Severe	Balls et al. (1995)
1-Naphthalene acetic acid, Na salt	61-31-4	3	100%	Solid	95	water soluble		4.90	Severe		Balls et al. (1995)
Octanol	111-87-5	1	100%	Liquid	>99	water insoluble		2.10	Severe	Moderate	Balls et al. (1995)
Octanol	111-87-5	2	100%	Liquid	>99	water insoluble		1.00	Nonirritant		Balls et al. (1995)
Octanol	111-87-5	3	100%	Liquid	>99	water insoluble		1.80	Moderate		Balls et al. (1995)
Octanol	111-87-5	4	100%	Liquid	>99	water insoluble		1.78	Moderate		Balls et al. (1995)
Parafluoraniline	371-40-4	1	100%	Liquid	99	water insoluble		5.25	Severe	Severe	Balls et al. (1995)
Parafluoraniline	371-40-4	2	100%	Liquid	99	water insoluble		4.46	Severe		Balls et al. (1995)
Parafluoraniline	371-40-4	3	100%	Liquid	99	water insoluble		1.90	Moderate		Balls et al. (1995)
Parafluoraniline	371-40-4	4	100%	Liquid	99	water insoluble		2.57	Severe		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	1	100%	Liquid		surfactant		1.59	Moderate	Nonirritant	Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	2	100%	Liquid		surfactant		0.72	Nonirritant		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	3	100%	Liquid		surfactant		0.60	Nonirritant		Balls et al. (1995)
Polyethylene glycol 400	25322-68-3	4	100%	Liquid		surfactant		1.22	Nonirritant		Balls et al. (1995)
Potassium cyanate	590-28-3	1	100%	Solid	97	water soluble		2.17	Severe	Severe	Balls et al. (1995)
Potassium cyanate	590-28-3	3	100%	Solid	97	water soluble		2.50	Severe		Balls et al. (1995)
Potassium cyanate	590-28-3	4	100%	Solid	97	water soluble		6.07	Severe		Balls et al. (1995)
Promethazine HCl	58-33-3	1	100%	Solid	100	water soluble		3.20	Severe	Severe	Balls et al. (1995)
Promethazine HCl	58-33-3	3	100%	Solid	100	water soluble		3.00	Severe		Balls et al. (1995)

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Pyridine	110-86-1	1	100%	Liquid	>99.9	water soluble		3.84	Severe	Severe	Balls et al. (1995)
Pyridine	110-86-1	2	100%	Liquid	>99.9	water soluble		7.76	Severe		Balls et al. (1995)
Pyridine	110-86-1	3	100%	Liquid	>99.9	water soluble		12.90	Severe		Balls et al. (1995)
Pyridine	110-86-1	4	100%	Liquid	>99.9	water soluble		10.44	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	1	1%	Solution		water soluble		6.34	Severe	Severe	Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	1%	Solution		water soluble		6.17	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	1%	Solution		water soluble		4.80	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	1%	Solution		water soluble		4.36	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	1	10%	Solution		water soluble		13.13	Severe	Severe	Balls et al. (1995)
Sodium hydroxide	1310-73-2	2	10%	Solution		water soluble		7.82	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	3	10%	Solution		water soluble		23.00	Severe		Balls et al. (1995)
Sodium hydroxide	1310-73-2	4	10%	Solution		water soluble		9.82	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	3%	Solution	98	surfactant		2.68	Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	3%	Solution	98	surfactant		1.62	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	3%	Solution	98	surfactant		1.70	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	3%	Solution	98	surfactant		2.46	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	1	15%	Solution	98	surfactant		2.86	Severe	Severe	Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	2	15%	Solution	98	surfactant		2.34	Severe		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	3	15%	Solution	98	surfactant		1.80	Moderate		Balls et al. (1995)
Sodium lauryl sulfate	151-21-3	4	15%	Solution	98	surfactant		4.37	Severe		Balls et al. (1995)
Thiourea	62-56-6	1	100%	Solid	>99	water soluble		1.31	Nonirritant	Nonirritant	Balls et al. (1995)
Thiourea	62-56-6	3	100%	Solid	>99	water soluble		0.50	Nonirritant		Balls et al. (1995)
Toluene	108-88-3	1	100%	Liquid	99	water insoluble		3.18	Severe	Severe	Balls et al. (1995)
Toluene	108-88-3	2	100%	Liquid	99	water insoluble		5.84	Severe		Balls et al. (1995)
Toluene	108-88-3	3	100%	Liquid	99	water insoluble		2.90	Severe		Balls et al. (1995)
Toluene	108-88-3	4	100%	Liquid	99	water insoluble		2.98	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	3%	Solution		water soluble		18.76	Severe	Severe	Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	3%	Solution		water soluble		9.15	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	3%	Solution		water soluble		9.90	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	3%	Solution		water soluble		5.33	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	1	30%	Solution		water soluble		14.39	Severe	Severe	Balls et al. (1995)
Trichloroacetic acid	76-03-9	2	30%	Solution		water soluble		9.96	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	3	30%	Solution		water soluble		13.10	Severe		Balls et al. (1995)
Trichloroacetic acid	76-03-9	4	30%	Solution		water soluble		11.81	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	1	5%	Solution	98	surfactant		2.66	Severe	Severe	Balls et al. (1995)
Triton X-100	9002-93-1	2	5%	Solution	98	surfactant		2.72	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	3	5%	Solution	98	surfactant		1.40	Nonirritant		Balls et al. (1995)
Triton X-100	9002-93-1	4	5%	Solution	98	surfactant		2.20	Severe		Balls et al. (1995)
Triton X-100	9002-93-1	1	10%	Solution	98	surfactant		3.45	Severe	Severe	Balls et al. (1995)
Triton X-100	9002-93-1	2	10%	Solution	98	surfactant		1.71	Moderate		Balls et al. (1995)
Triton X-100	9002-93-1	3	10%	Solution	98	surfactant		1.70	Moderate		Balls et al. (1995)
Triton X-100	9002-93-1	4	10%	Solution	98	surfactant		2.40	Severe		Balls et al. (1995)
Tween 20	9005-64-5	1	100%	Liquid	98	surfactant		0.39	Nonirritant	Nonirritant	Balls et al. (1995)
Tween 20	9005-64-5	2	100%	Liquid	98	surfactant		0.38	Nonirritant		Balls et al. (1995)
Tween 20	9005-64-5	3	100%	Liquid	98	surfactant		0.60	Nonirritant		Balls et al. (1995)
Tween 20	9005-64-5	4	100%	Liquid	98	surfactant		0.95	Nonirritant		Balls et al. (1995)

Abbreviation: CASRN = Chemical Abstract Service Registry Number, HCl = Hydrochloric acid.

¹ Solubility obtained from literature references, where available, expressed as g/mL.² Q-Score represents irritation scores that were calculated using the method described in Balls et al. (1995)